

4-Pentenoic acid, 2-methyl-, heptyl ester

Inchi:	InChI=1S/C13H24O2/c1-4-6-7-8-9-11-15-13(14)12(3)10-5-2/h5,12H,2,4,6-11H2,1,3H3
InchiKey:	YYWMOBAOYMHVJR-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	C=CCC(C)C(=O)OCCCCCCC
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-89.94	kJ/mol	Joback Method
hf	-436.30	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.712		Crippen Method
mvol	197.170	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1411.00		NIST Webbook
tb	569.37	K	Joback Method
tc	743.83	K	Joback Method
tf	291.67	K	Joback Method
vc	0.762	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.52	J/molxK	569.37	Joback Method
cpg	568.51	J/molxK	714.75	Joback Method
cpg	555.03	J/molxK	685.68	Joback Method
cpg	540.91	J/molxK	656.60	Joback Method
cpg	526.12	J/molxK	627.52	Joback Method
cpg	510.67	J/molxK	598.45	Joback Method
cpg	581.36	J/molxK	743.83	Joback Method
dvisc	0.0001648	Paxs	569.37	Joback Method

dvisc	0.0002205	Paxs	523.09	Joback Method
dvisc	0.0003123	Paxs	476.80	Joback Method
dvisc	0.0004767	Paxs	430.52	Joback Method
dvisc	0.0008057	Paxs	384.24	Joback Method
dvisc	0.0015720	Paxs	337.95	Joback Method
dvisc	0.0037924	Paxs	291.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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